Diphenylurea

102-07-8 | DTXSID2025183

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 269 °C

Global applicability domain: Outside

Local applicability domain index: 2.15e-01

Confidence level: 6.97e-01

Nearest Neighbors from the Training Set

Image not found
Diphenylurea
Measured: 262
Predicted: 269

Image not found
N-(4-Bromophenyl)urea
Measured: 260
Predicted: 256

Image not found
1-Phenylurea
Measured: 238
Predicted: 247

Image not found
Benzoic acid, 2-phenylhydrazide
Measured: 314
Predicted: 306

Image not found
Carbaryl
Measured: 315
Predicted: 297